

What is claimed is:

1. A method for segregating compounds by ionization polarity for use in polarity sensitive analysis thereof, said method comprising the steps of:

5 a) selecting a data base of a statistically significant group of compounds and determining the polarization, positive or negative, at which each of said compounds is ionized;

10 b) structurally analyzing the individual compounds to determine structural characteristics common to a majority of compounds which ionize at positive polarity and to determine structural characteristics common to a majority of compounds which ionize at negative polarity, as polarization determinants;

c) sequentially arranging the polarization determinants in classification trees according to percentage determination of one of said negative or positive polarization;

15 d) applying the polarization determinants in one of said classification trees in classifying a new compound for a predicted polarization of positive or negative at which said compound is ionized;

e) segregating compounds classified as ionizing at positive polarity and compounds classified as ionizing at negative polarity; and

20 f) separately analyzing the segregated compounds with the respective predicted polarities with an analysis instrument operable in different modes depending on ionization polarity.

2 The method of claim 1, wherein said analysis instrument is a mass spectrometer.

3 The method of claim 2, wherein a polarization determinant is the presence of an OH group.

25 4 The method of claim 2, wherein a polarization determinant is one of the presence of more than two oxygen atoms and the presence of less than two oxygen atoms.

5 The method of claim 4, wherein the presence of more than two oxygen atoms or the presence of less than two oxygen atoms is a determinant, if an OH group is present.

30 6 The method of claim 5, wherein, in the absence of an OH group, the presence or absence of CH_2QCH_2 groups, where Q is neither C or H, is a discriminator of polarity.